Samuela Pasquali

List of Publications by Year
in descending order

26 papers	1,579 citations	516710 16 h-index	580821 25 g-index
29 all docs	29 docs citations	29 times ranked	1823 citing authors

#	Article	IF	Citations
1	Investigating the structural changes due to adenosine methylation of the Kaposiâ€™s sarcoma-associated herpes virus ORF50 transcript. PLoS Computational Biology, 2022, 18, e1010150.	3.2	8
2	RNA Modeling with the Computational Energy Framework. Methods in Molecular Biology, 2021, 2323, 49-66.	0.9	4
3	Induced forms of Î±2-macroglobulin neutralize heparin and direct oral anticoagulant effects. International Journal of Biological Macromolecules, 2021, 184, 209-217.	7.5	4
4	Biasing RNA Coarse-Grained Folding Simulations with Small-Angle X-ray Scattering Data. Journal of Chemical Theory and Computation, 2021, 17, 6509-6521.	5.3	12
5	Structural transitions in the RNA 7SK 5â€² hairpin and their effect on HEXIM binding. Nucleic Acids Research, 2020, 48, 373-389.	14.5	15
6	Molecular modelling as the spark for active learning approaches for interdisciplinary biology teaching. Interface Focus, 2019, 9, 20180065.	3.0	11
7	Coarse-grained dynamic RNA titration simulations. Interface Focus, 2019, 9, 20180066.	3.0	15
8	Protein-RNA complexation driven by the charge regulation mechanism. Biochemical and Biophysical Research Communications, 2018, 498, 264-273.	2.1	29
9	Ten simple rules to create a serious game, illustrated with examples from structural biology. PLoS Computational Biology, 2018, 14, e1005955.	3.2	20
10	The crystal structure of the 5â€² functional domain of the transcription riboregulator 7SK. Nucleic Acids Research, 2017, 45, gkw1351.	14.5	25
11	What Can Human-Guided Simulations Bring to RNA Folding?. Biophysical Journal, 2017, 113, 302-312.	0.5	8
12	Multifunctional energy landscape for a DNA G-quadruplex: An evolved molecular switch. Journal of Chemical Physics, 2017, 147, 152715.	3.0	32
13	Coarse-Grained Simulations Complemented by Atomistic Molecular Dynamics Provide New Insights into Folding and Unfolding of Human Telomeric G-Quadruplexes. Journal of Chemical Theory and Computation, 2016, 12, 6077-6097.	5.3	50
14	Electrostatics analysis of the mutational and pH effects of the N-terminal domain self-association of the major ampullate spidroin. Soft Matter, 2016, 12, 5600-5612.	2.7	38
15	UnityMol: interactive and ludic visual manipulation of coarse-grained RNA and other biomolecules. , 2015, , .		7
16	Ab initioRNA folding. Journal of Physics Condensed Matter, 2015, 27, 233102.	1.8	16
17	Coarse-Grained HiRE-RNA Model for ab Initio RNA Folding beyond Simple Molecules, Including Noncanonical and Multiple Base Pairings. Journal of Chemical Theory and Computation, 2015, 11, 3510-3522.	5.3	65
18	Amyloid Î² Protein and Alzheimerâ€™s Disease: When Computer Simulations Complement Experimental Studies. Chemical Reviews, 2015, 115, 3518-3563.	47.7	530

#	Article	IF	Citations
19	The OPEP protein model: from single molecules, amyloid formation, crowding and hydrodynamics to DNA/RNA systems. Chemical Society Reviews, 2014, 43, 4871-4893.	38.1	147
20	Coarse-Grained Simulations of RNA and DNA Duplexes. Journal of Physical Chemistry B, 2013, 117, 8047-8060.	2.6	77
21	The Coarse-Grained OPEP Force Field for Non-Amyloid and Amyloid Proteins. Journal of Physical Chemistry B, 2012, 116, 8741-8752.	2.6	98
22	Impact of Thermostats on Folding and Aggregation Properties of Peptides Using the Optimized Potential for Efficient Structure Prediction Coarse-Grained Model. Journal of Chemical Theory and Computation, 2011, 7, 1502-1510.	5.3	20
23	HiRE-RNA: A High Resolution Coarse-Grained Energy Model for RNA. Journal of Physical Chemistry B, 2010, 114, 11957-11966.	2.6	113
24	Modular RNA architecture revealed by computational analysis of existing pseudoknots and ribosomal RNAs. Nucleic Acids Research, 2005, 33, 1384-1398.	14.5	26
25	Exploring the repertoire of RNA secondary motifs using graph theory; implications for RNA design. Nucleic Acids Research, 2003, 31, 2926-2943.	14.5	139
26	Analysis of Protein Sequence/Structure Similarity Relationships. Biophysical Journal, 2002, 83, 2781-2791.	0.5	70